



```

chain nodes :
5 12 13 14 15 16 17 18 19 20 21 22 23 24 25 30 32
ring nodes :
1 2 3 4 6 7 8 9 10 11
chain bonds :
1-12 2-5 4-30 4-32 5-6 5-16 13-15 13-14 13-17 18-19 18-21 19-20 22-23
23-24 23-25
ring bonds :
1-2 1-4 2-3 3-4 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-4 1-12 2-3 2-5 3-4 4-30 4-32 5-16 13-15 13-14 13-17 18-19 19-20
22-23 23-24 23-25
exact bonds :
5-6 18-21
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11

```

G1:NH2, [*1], [*2], [*3]

G2:H, CN, COOH, Ak, Cb

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:CLASS 18:CLASS
19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 30:CLASS 32:CLASS

```

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:48:50 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2318 TO ITERATE

86.3% PROCESSED 2000 ITERATIONS

3 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 43473 TO 49247

PROJECTED ANSWERS: 3 TO 180

L2 3 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 11:48:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 46493 TO ITERATE

100.0% PROCESSED 46493 ITERATIONS

82 ANSWERS

SEARCH TIME: 00.00.01

L3 82 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'HCAPLUS' ENTERED AT 11:48:58 ON 25 FEB 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Andrew Freistein 10/804,558

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FILE LAST UPDATED: 24 Feb 2006 (20060224/ED)

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3

L4 13 L3

=> d ibib hitstr 2-13